TOPIC 12 – ATOMIC STRUCTURE (HL)12.1 – ELECTRON CONFIGURATION

IB Chemistry

T02D05

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12.1 – Electron Configuration

- 12.1.1 Explain how evidence from first ionization energies across periods accounts for the existence of main energy levels and sub-levels in atoms. (3)
- 12.1.2 Explain how successive ionization energy data is related to the electron configuration of an atom. (3)
- 12.1.3 State the relative energies of s, p, d and f orbitals in a single energy level. (1)
- 12.1.4 State the maximum number of orbitals in a given energy level. (1)
- 12.1.5 Draw the shape of an s orbital and the shapes of the px, py and pz orbitals. (1)
- 12.1.6 Apply the Aufbau principle, Hund's rule and the Pauli exclusion principle to write electron configurations for atoms and ions up to Z = 54. (2)

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12.1.1 – Ionization Energy

- 12.1.1 Explain how evidence from first ionization energies across periods accounts for the existence of main energy levels and sub-levels in atoms. (3)
- The **first ionization energy** is the minimum energy per mole required to remove electrons from one mole of isolated gaseous atoms to form one mole of gaseous unipositive ions under standard thermodynamic conditions.
  - $Cl(g) \rightarrow Cl^{+}(g) + e^{-}$

12.1 – Factors affecting I.E.

- Factors that affect the ionization energy
  - The size of the atom (or ion)
    - As the size increases the nucleus becomes farther from the outermost electrons, and the attraction between the two falls
  - The nuclear charge
    - As the nuclear charge become positive (more p) its attraction to the electrons increases. **Effective nuclear charge** is a large impact
  - The **shielding** effect
    - The outer e^- are repelled by the other e^- in the atom and shields the valence electrons from the nucleus

12.1.2 – I.E. Data

- 12.1.2 Explain how successive ionization energy data is related to the electron configuration of an atom. (3)
  - The concept of successive ionization energies (1^{st}, 2^{nd}, 3^{rd}, etc) will be explored further in periodicity.

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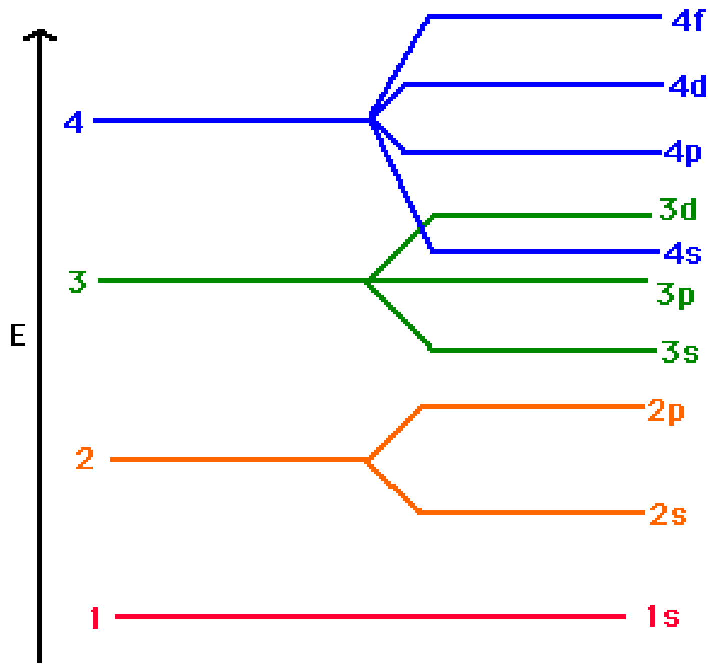
12.1.3 – Orbital Filling Order

- 12.1.3 State the relative energies of s, p, d and f orbitals in a single energy level. (1)
- The energy of the sub-levels increases from s to p to d to f. The electrons fill up the lower energy sub-levels first.



Looking at this table can you work out in what order the electrons fill the sub-levels?

Energy Levels

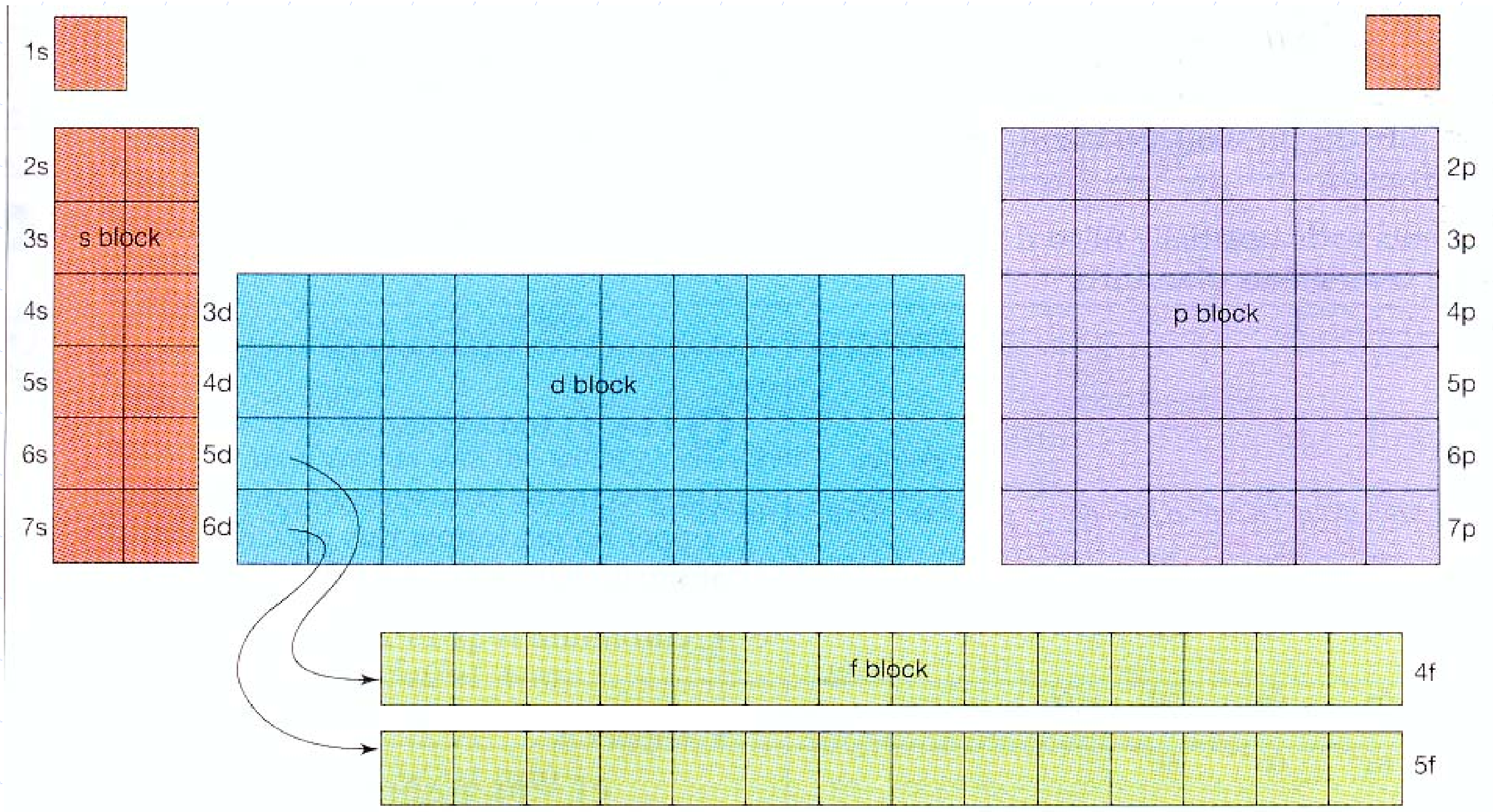
- Electrons go in shells or energy levels. The energy levels are called **principle energy levels**, 1 to 4. (known as n=1, n=2, etc)
- The energy levels contain sub-levels.

Principle energy level	Number of sub-levels
1	1
2	2
3	3
4	4

These sub-levels are assigned the letters, s, p, d, f

12.1.4 – Max Orbitals, Why?

- 12.1.4 State the maximum number of orbitals in a given energy level. (1)



12.1.4 - Energy Levels

- Each type of sub-level (shape) can hold a different maximum number of electrons and orbitals.

Sub-level	Maximum number of orbitals	Maximum number of electrons
s	1	2
p	3	6
d	5	10
f	7	14

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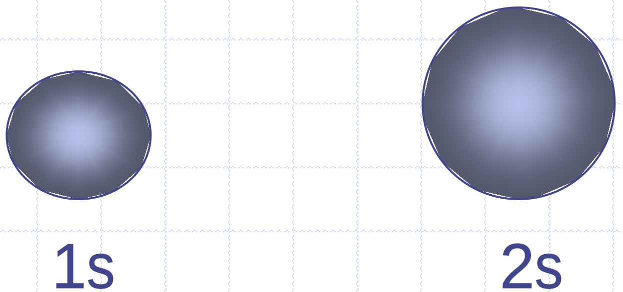
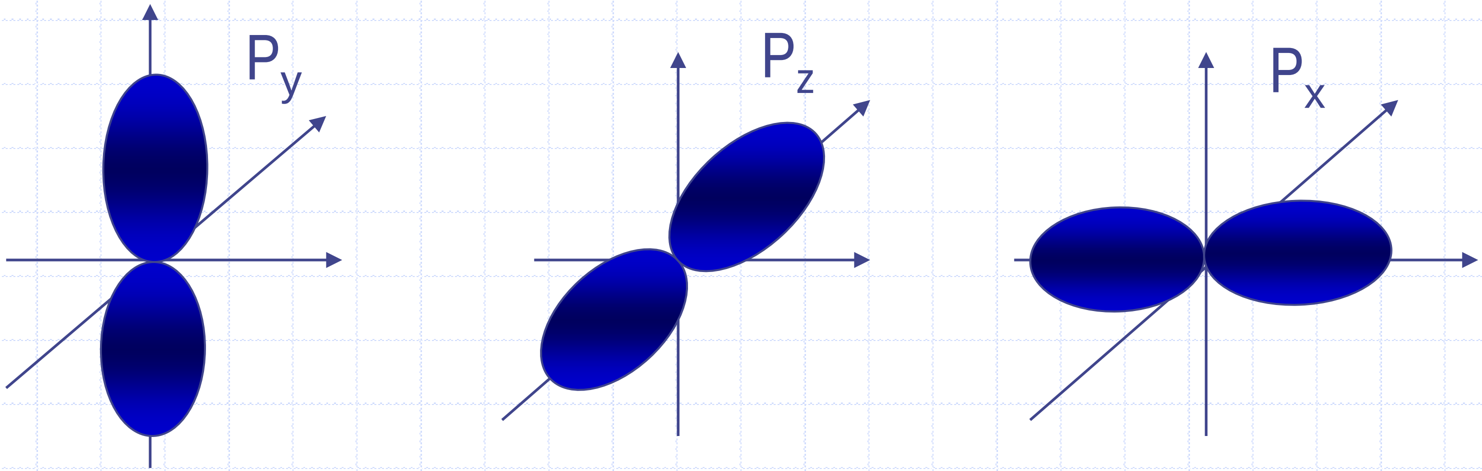
12.1.5 - Models

- 12.1.5 Draw the shape of an s orbital and the shapes of the px, py and pz orbitals. (1)

  - **s orbitals**



  - **p orbitals**



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12.1.5 - What do d, f...look like?

- Remember, these orbitals represent mathematical calculations of where electrons (behaving wave-like) reside.
- The calculation is a probability. As the equation calculates probability further from the nucleus the equations and space-filling representations become very...... funky.
- Probability Clouds

12.1.6 – E. Configurations and Box Diagrams

- 12.1.6 Apply the Aufbau principle, Hund's rule and the Pauli exclusion principle to write electron configurations for atoms and ions up to Z = 54. (2)
  - Electron Configuration:

$1s^2$

Energy level

Sub-level

Number of electrons

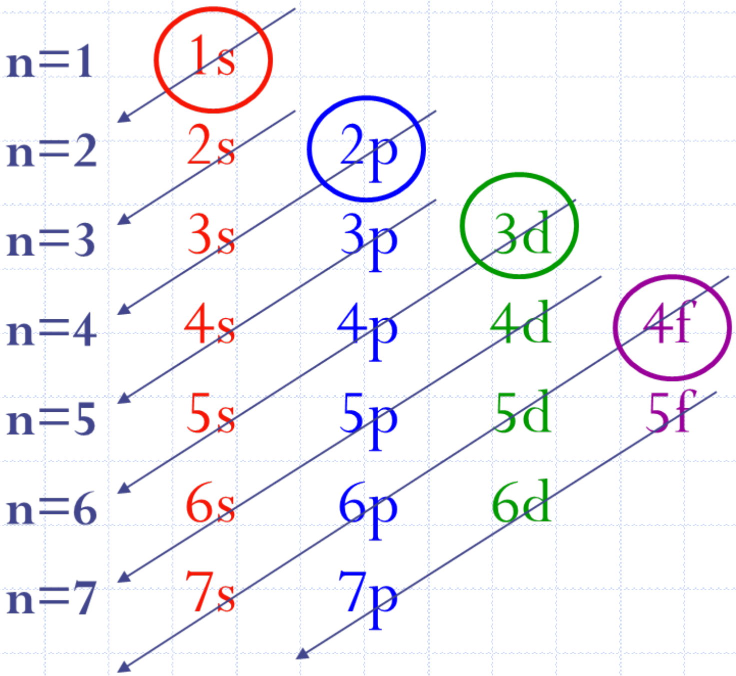
<u>Example</u>

For magnesium:

$1s^2, 2s^2, 2p^6, 3s^2$

12.1.6 - Electronic Structure

- The electronic structure follows a pattern – the order of filling the sub-levels is 1s, 2s, 2p, 3s, 3p...
- The order in which the energy levels are filled is called the Aufbau Principle.
- After this there is a break in the pattern, as that the 4s fills before 3d. – Use the following diagram to help:



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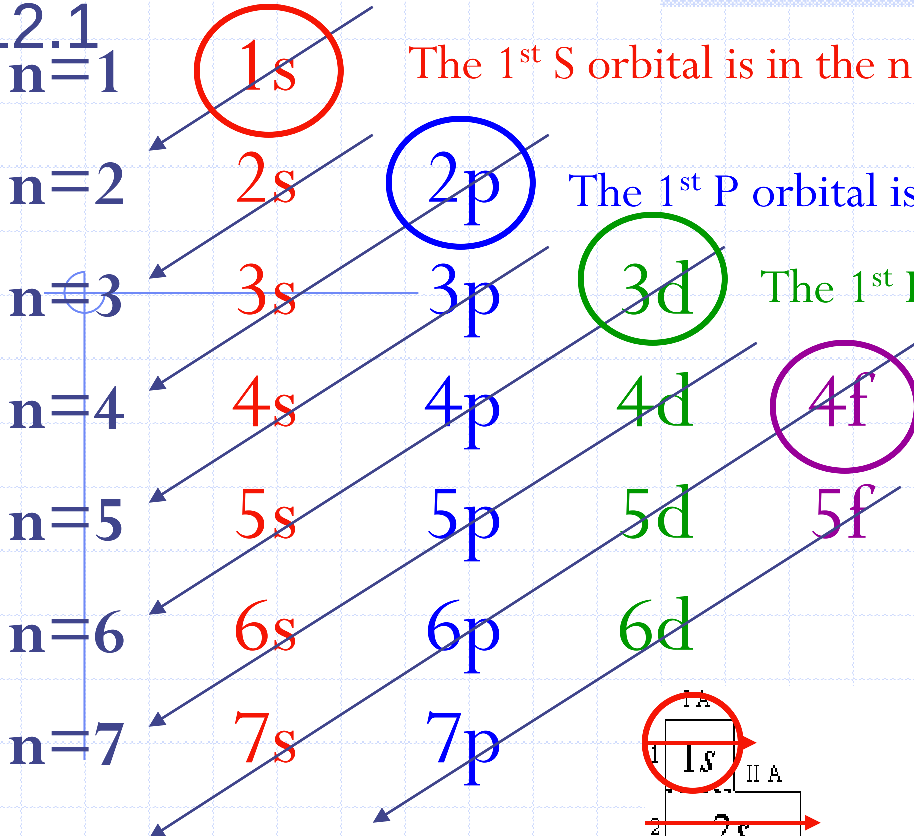
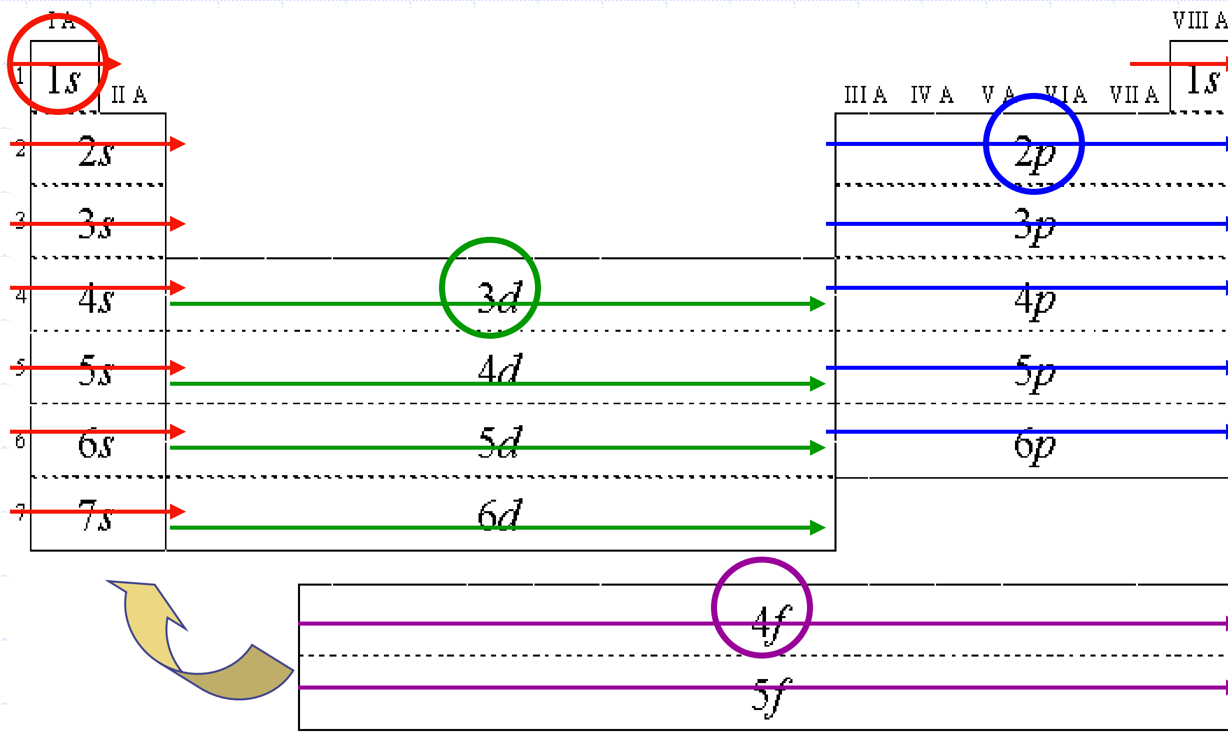
The 1st S orbital is in the n=1 energy level

The 1st P orbital is in the n=2 energy level

The 1st D orbital is in the n=3 energy level

The 1st F orbital is in the n=4 energy level





[Filling Order of Orbitals (link)]

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12.1.6 - Electronic Structure

- There are two exceptions to the Aufbau principle for neutral elements (more for ions).
- The electronic structures of chromium and copper do not follow the pattern – they are anomalous.
- Why is this, because of **Hund's rule** (you'll see)
- Chromium – $1s^2$, $2s^2$, $2p^6$, $3s^2$, $3p^6$, $3d^5$, $4s^1$
- Copper – $1s^2$, $2s^2$, $2p^6$, $3s^2$. $3p^6$, $3d^{10}$, $4s^1$

Write the electronic configuration for the following elements:

a) hydrogen
b) carbon
c) oxygen
d) aluminium
e) copper
f) fluorine

Electronic Structure – of ions

- When an atom loses or gains electrons to form an ion, the electronic structure changes:
  - Positive ions: formed by the loss of e^-

$$1s^2\ 2s^2\ 2p^6\ 3s^1 \rightarrow 1s^2\ 2s^2\ 2p^6$$

Na atom **Na^+ ion**

  - Negative ions: formed by the gain of e^-

$$1s^2\ 2s^2\ 2p^4 \rightarrow 1s^2\ 2s^2\ 2p^6$$

O atom **O^{2-} ion**

Electronic Structure – of transition metals

- With the transition metals it is the **4s** electrons that are lost first when they form ions:
  - Titanium (Ti) - loss of 2 e^-

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^2\ \mathbf{4s^2} \rightarrow 1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^2$

Ti atom **Ti^{2+} ion**

  - Chromium (Cr) - loss of 3 e^-

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^5\ \mathbf{4s^1} \rightarrow 1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^3$

Cr atom **Cr^{3+} ion**

Electronic Structure - Questions

- Give the full electronic structure of the following positve ions:

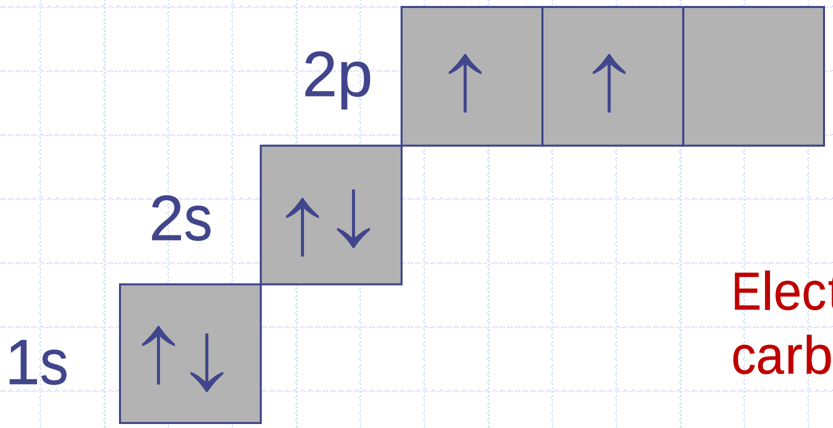
  a) Mg^{2+} b) Ca^{2+} c) Al^{3+}

- Give the full electronic structure of the negative ions:

  a) Cl^{-} b) Br^{-} c) P^{3-}

Orbitals

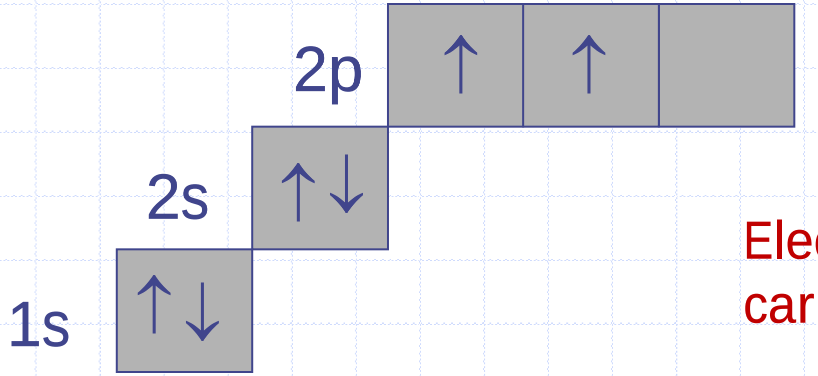
- Within a sub-level, the electrons occupy orbitals as unpaired electrons rather than paired electrons. (This is known as **Hund's Rule**).
- We use boxes to represent orbitals:



Electronic structure of carbon, $1s^2$, $2s^2$, $2p^2$

Orbitals

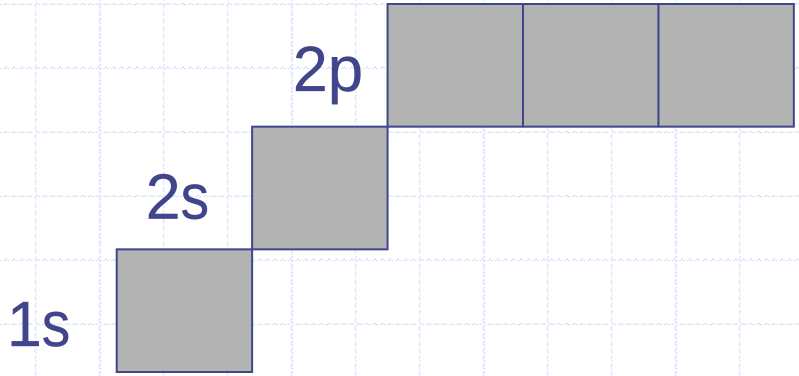
- The arrows represent the electrons in the orbitals.
- The direction of arrows indicates the spin of the electron.
- Paired electrons will have opposite spin, as this reduces the **mutual repulsion** between the paired electrons. This is known as the **Pauli Exclusion Principle**



Electronic structure of carbon, $1s^2$, $2s^2$, $2p^2$

Orbitals

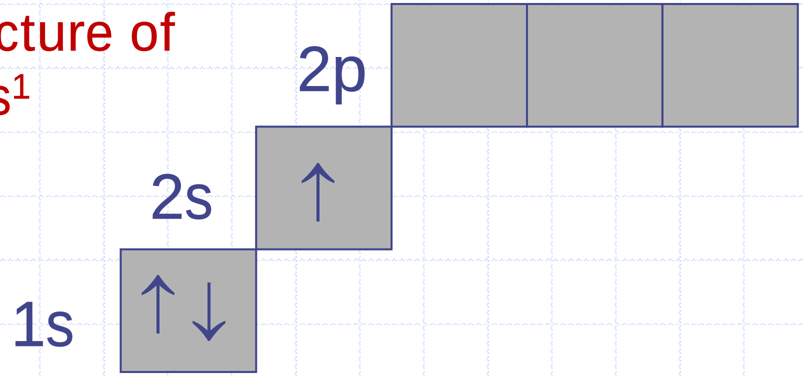
- Using boxes to represent orbitals, give the full electronic structure of the following atoms:
  - a) lithium
  - b) fluorine
  - c) potassium
  - d) nitrogen
  - e) oxygen



Orbitals

- Using boxes to represent orbitals, give the full electronic structure of the following atoms:
  a) lithium b) fluorine c) potassium
  d) nitrogen e) oxygen

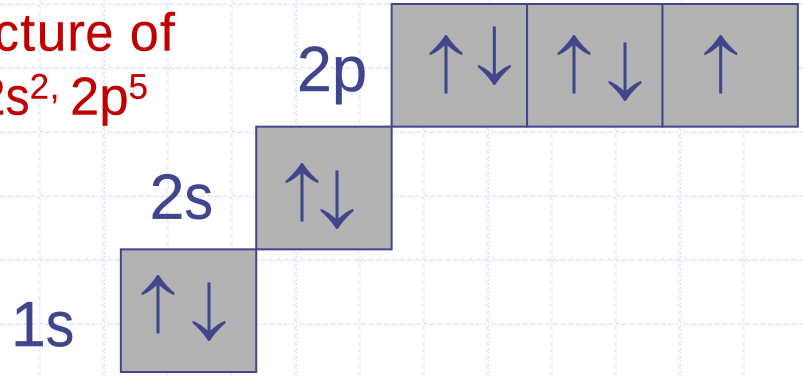
Electronic structure of lithium: $1s^2$, $2s^1$



Orbitals

- Using boxes to represent orbitals, give the full electronic structure of the following atoms:
  - a) lithium
  - b) fluorine
  - c) potassium
  - d) nitrogen
  - e) oxygen

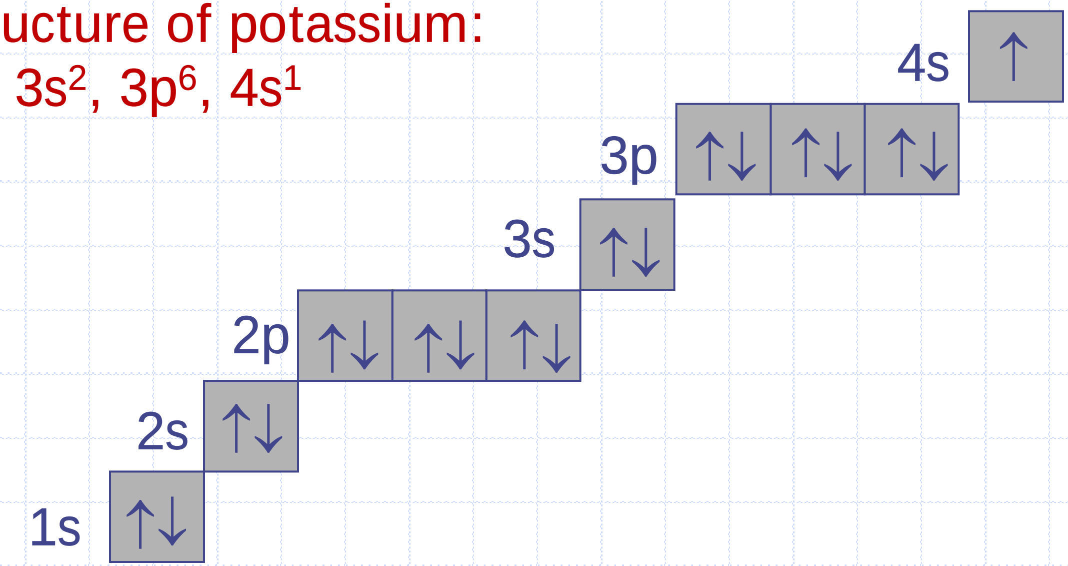
Electronic structure of fluorine: $1s^2$, $2s^2$, $2p^5$



Orbitals

- Using boxes to represent orbitals, give the full electronic structure of the following atoms:
  - a) lithium
  - b) fluorine
  - c) potassium
  - d) nitrogen
  - e) oxygen

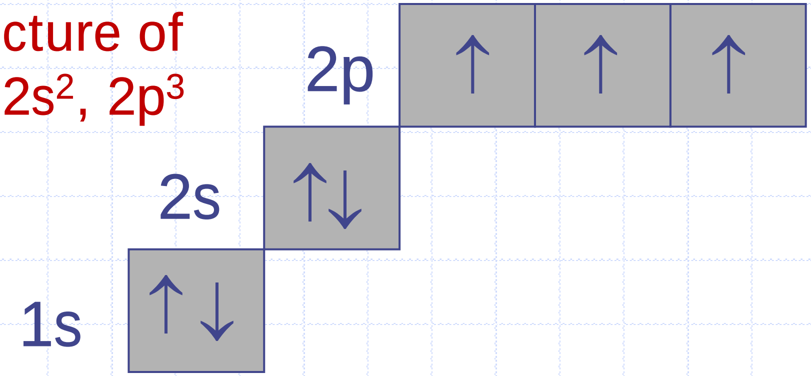
Electronic structure of potassium:
$1s^2, 2s^2, 2p^6, 3s^2, 3p^6, 4s^1$



Orbitals

- Using boxes to represent orbitals, give the full electronic structure of the following atoms:
  - a) lithium
  - b) fluorine
  - c) potassium
  - d) nitrogen
  - e) oxygen

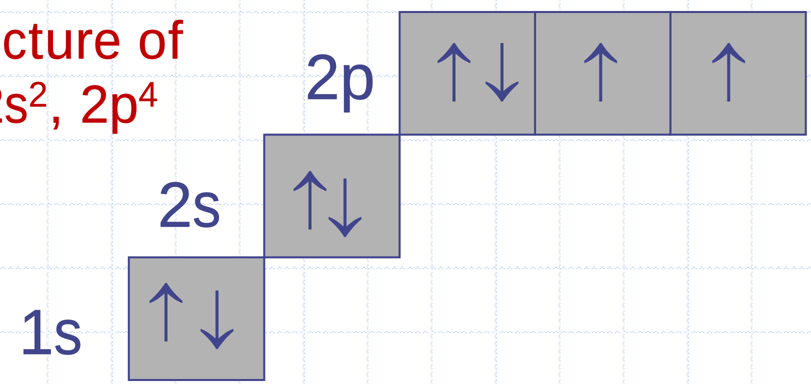
Electronic structure of nitrogen: $1s^2$, $2s^2$, $2p^3$



Orbitals

- Using boxes to represent orbitals, give the full electronic structure of the following atoms:
  - a) lithium
  - b) fluorine
  - c) potassium
  - d) nitrogen
  - e) oxygen

Electronic structure of oxygen: $1s^2$, $2s^2$, $2p^4$



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